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Effective Two-Body Method for Two-Electron Atoms

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EFFECTIVE TWO-BODY METHOD FOR TWO-ELECTRON ATOMS

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Abstract

The purpose of this note is to investigate some possibilities of obtaining in a simple manner approximate solutions of the bound two-electron atomic system. In particular, an effective two-body method is studied. It consists essentially of the assumption of a simple functional form for the wave function. The resulting Schrödinger equation may be solved exactly, yielding upper bounds of all the eigenvalues of the system. Only the lowest approximate eigenvalue is near to the exact result. Some methods of improvement are suggested and discussed.

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1. Introduction

In the present note we wish to present some observations on the non-relativistic two-electron atomic system. We hope these may prove useful and stimulating to additional efforts to obtain approximate eigenfunctions and eigenvalues. In particular, we examine the reduction of the problem to an "effective two-body" system, an idea that has been used in the corresponding three-body nuclear system, the triton[1], [2]. A complete review of the extensive treatment of the two-electron atomic system, in particular the helium atom, may be found in the recent book of Bethe and Salpeter[3]. The variational formulation of the problem, which is the basis of the present investigation, is reviewed here.

Instead of the electronic radial coordinates r_1, r_2 and the electronic interdistance r_{12}, it has been found convenient in the past to use the variables

$$s = r_1 + r_2 \; ; \quad t = r_2 - r_1 \; ; \quad u = r_{12} \tag{1}$$

The variational principle for the Schrödinger equation for a two-electron atom in a state of zero total angular momentum may be written as

$$\delta \int (\psi H \psi - E\psi^2)\, d\tau = 0 \tag{2}$$

where

$$\int \psi H \psi\, d\tau = \int_0^{\infty} ds \int_0^{s} du \int_{-u}^{u} dt \left\{ (s^2-t^2)u\left[\left(\frac{\partial\psi}{\partial s}\right)^2 + \left(\frac{\partial\psi}{\partial t}\right)^2 + \left(\frac{\partial\psi}{\partial u}\right)^2\right] + 2s(u^2-t^2)\frac{\partial\psi}{\partial s}\frac{\partial\psi}{\partial u} + 2t(s^2-u^2)\frac{\partial\psi}{\partial t}\frac{\partial\psi}{\partial u} + (s^2-t^2-4Zsu)\psi^2 \right\}, \tag{3}$$

$$\int \psi^2\, d\tau = \int_0^{\infty} ds \int_0^{s} du \int_{-u}^{u} dt\,(s^2-t^2)u\psi^2 \quad , \tag{4}$$

and

(5) $$\psi = \psi(s,t,u) \ .$$

The parameter Z is the charge number of the nucleus, for example, Z = 2 for the helium atom. The units are those of Hartree: m = 1, e = 1, $\frac{\hbar^2}{me^2} = a_o = 1$. In these units, the ground state energy of the hydrogen atom is $(-\frac{1}{2})$. The unit of energy in electron volts is 27.1.

The most accurate calculations on the ground state of the helium atom have utilized the Ritz variational form of the energy with the insertion of appropriate trial wave functions ψ_t. If the electronic interaction (the term $(s^2-t^2)\psi^2$ in equation (3)) were absent, the exact ground state wave function would be the product of two hydrogenic ground state wave functions

(6) $$\psi_o = e^{-Zr_1} \cdot e^{-Zr_2} = e^{-Zs} \ .$$

Consequently, in one of his very early calculations, Hylleraas[4] chose ψ_o as a trial function with Z a variational parameter, and obtained the best value Z = 27/16, for which

(7) $$E_o = -2.85\_ \ .$$

This is already within 2 % of the experimental value of the parahelium ('S) ground state,

(8) $$E_{o\ exp} = -2.904 \ .$$

Many efforts by Hylleraas and others have been made to improve this result by assuming the trial functions to be of the form

(9) $$\psi_t = e^{-ks} \sum c_{\ell,m,n} s^{\ell} u^m t^n$$

with k and $c_{\ell,m,n}$ as variational parameters. The most ambitious calculation along these lines was performed recently by Kinoshita[5] who utilized a series of 38 terms. His result for the lowest energy value is

$$E_o = -\,2.9037225\ . \tag{10}$$

Such calculations require an extensive amount of labor. In looking into this problem, we were motivated by a desire to obtain approximate solutions of the two-electron system with little computational effort.

2. The effective two-body method

In particular, we have applied the technique of converting the three-body problem to an effective two-body problem which has been utilized in the investigation of the binding energy of the triton, the corresponding three-body nuclear problem[1], [2]. The restriction of ψ_t to be a function of only one variable effects such a conversion. Thus, if we let $\psi_t = \phi(s)$ only, the variational principle (1) reduces to

$$\delta \int_0^\infty ds \left\{ \frac{8}{30}\, s^5 (\phi')^2 - \frac{(16Z-5)}{12}\, s^4 \phi^2 - \frac{8}{30}\, E\, s^5 \phi^2 \right\} = 0. \tag{11}$$

The Euler-Lagrange equation for $\phi(s)$ is then

$$\frac{1}{s^5}\,\frac{d}{ds}\left(s^5\,\frac{d\phi}{ds}\right) + \frac{5}{16}\,\frac{(16Z-5)}{s}\,\phi + E\phi = 0\ . \tag{12}$$

So far all this was observed by Hylleraas, who also noted that the lowest eigenfunction and eigenvalues are given by equations (6) and (7), respectively. It does not appear to have been noticed previously that (12) may be solved for all its eigenfunctions and eigenvalues. Setting $\phi(s) = s^{-3/2}F(s)$, the equation for F becomes

$$\frac{d^2F}{ds^2} + \frac{2}{s}\,\frac{dF}{ds} + \left(E + \frac{2\zeta}{s} - \frac{\lambda(\lambda+1)}{s^2}\right)F = 0 \tag{13}$$

with $\zeta = \frac{5}{32}(16Z-5)$ and $\lambda = 3/2$.

This is readily recognized as the hydrogenic equation (see Appendix). Consequently, F is to be interpreted as an " effective" two-body wave function representing a hydrogenic system for which the charge on the nucleus is ζ and the effective orbital quantum number is λ. The non-singular eigenfunctions of this equation are simple generalizations of the usual hydrogenic solutions and may be written as

$$(14) \qquad F_n = \rho^{\lambda} e^{-\frac{\rho}{2}} L_n^{\lambda}(\rho) , \qquad \rho = 2ks, \qquad k^2 = |E| ,$$

with $L_n^{\lambda}(\rho)$ the generalized Lagrange function (See Appendix). In particular, $F_0 = \rho^{3/2} e^{-\rho/2}$. The associated eigenvalues, just as in the hydrogen problem, are

$$(15) \qquad E_n = - \frac{\zeta^2}{(n+\lambda+1)^2} , \qquad n = 0,1,2....$$

It is known that for each n, the n-th largest eigenvalue of a matrix which is reduced by one row and column is an upper bound on the n-th largest eigenvalue of the original matrix. This theorem was first applied in the present variational context by Hylleraas and Undheim[6], and it follows that the above eigenvalues are respective upper bounds of the true 'S eigenvalues of the two-electron system. Furthermore, the eigenfunctions form a complete orthogonal set in the variable s over the domain $(0,\infty)$. This result for the ground state eigenvalue E_0 compares well with the experimental values, as may be seem in Table I. The values of the lowest eigenvalues for all two-electron atoms from $Z = 1$ to $Z = 9$ are given there.

Naturally these same results could have been obtained by choosing as a trial function a simple exponential. We may, however, make the stronger assertion that the exponential form is the 'best' function which is exclusively a function of s. This observation is independent of the value of Z; in fact we see that explicit minimization with respect to Z has been

Atom	H^-	He	Li^+	Be^{++}	B^{+++}	C^{++}	N^{5+}	O^{6+}	F^{7+}
Z	1	2	3	4	5	6	7	8	9
Effective charge ζ	1.72	4.22	6.72	9.22	11.72	14.22	16.72	19.22	21.72
$-E_o$ Eq.(15)	473	2.848	7.223	13.598	21.973	32.348	44.723	59.098	75.473
$-\alpha$	+0.265	+.137	.09	.07	.06	.05	.04	.04	.03
$-E_o$ Eq.(18)	0.507901	2.889618	7.2668	13.6429	22.0183	32.3937	44.7693	59.1436	75.5196
$-E_o$ exp.	.5275	2.904	7.280	13.657	22.035	32.417	44.802	59.194	75.56

Table I.

A comparison of the ground state eigenvalue as given by equations (15) and (18), and the experimental values as given by Moore[7] for all atoms from Z = 1 to Z = 9.

avoided. It may also be observed from Table I that the discrepancy from the experimental result is more or less constant with Z so that, percentagewise, this error becomes more negligible as Z increases. Conversely, the value for H^- (Z=1) is not even sufficient to bind the second electron because E_o is greater than $(-\frac{1}{2})$. The values obtained for the second state are uniformly poor: for all Z the second state is given as $E_1 = (\frac{25}{49})E_o$ and this value is never below the energy level of a single electron attached to a nucleus with charge Z. Thus, the effective two-body approximation introduces a special simplicity which may be considered a good approximation to the true wave function only for the ground state. Nevertheless, the ^1S solutions may be useful not only in providing a complete orthogonal set of functions in the variable s, but also in indicating the "best" form of the eigenfunctions in their dependence on s.

3. Introduction of a free parameter

The ease with which it is possible to obtain these approximate solutions makes it appear desirable to search for ways of improving the accuracy while still retaining the ease of solution of the resulting two-body Schrödinger equation. One way of accomplishing this is to introduce the variable $S = s+\alpha u$ instead of s, where α is an arbitrary parameter. The volume element now becomes

$$(16) \qquad \int d\tau = \int_o^\infty dS \int_o^{S/1+\alpha} du \int_{-u}^{u} dt \left[(S-\alpha u)^2 - t^2\right] u \quad \text{with} \quad \alpha > -1 \, .$$

Assume now that $\psi_t = \phi(S)$ only. We may again integrate over u and t to obtain

$$(17) \qquad \delta \int_o^\infty dS \left\{ a(\alpha) \frac{8}{30} S^5 \left(\frac{d\phi}{dS}\right)^2 - v(\alpha,Z) \frac{16Z-5}{12} S^4 \phi^2 + n(\alpha) \frac{8}{30} E \, S^5 \phi^2 \right\} = 0$$

where $\qquad a(\alpha) = \frac{1}{8}(8 + 15\alpha + 11\alpha^2 + 5\alpha^3 + \alpha^4)$

$$v(\alpha,Z) = \frac{1+\alpha}{16Z-5}\left[16Z-5+4(Z-1)\alpha-\alpha^2\right]$$

$$n(\alpha) = \frac{1}{8}(8+5\alpha+\alpha^2) \ .$$

Clearly, setting $\alpha = 0$ reduces this equation to the one previously considered. Furthermore, the eigenfunctions and eigenvalues are the same as before provided we substitute $\zeta(Z)\,\frac{v(\alpha,Z)}{a(\alpha)}$ for ζ and $E\,\frac{n(\alpha)}{a(\alpha)}$ for E. The eigenvalues are therefore given as

$$(18) \qquad E_n = -\left[\frac{5}{16}\,\frac{(16Z-5)}{(2n+5)}\right]^2 \frac{v^2(\alpha,Z)}{a(\alpha)n(\alpha)} \ .$$

The eigenvalues are again

$$(19) \qquad \phi_n = e^{-\rho/2}L_n^{\lambda}(\rho)$$

with

$$\rho = 2k_nS \quad \text{and} \quad k_n^2 = \left|\frac{n(\alpha)}{a(\alpha)}\,E_n\right| .$$

This expression for E_n may be minimized with respect to α, because it still constitutes a statinnary expression for E_n. For helium, the best value of α is

$$(20) \qquad \begin{cases} & \alpha = -\ 0.137 \\ \text{for which} & E_o = -\ 2.889618 \\ \text{and} & \phi_o = e^{-k_o(s-0.137u)} \ . \end{cases}$$

Of course, this duplicates the result of Hylleraas obtained with the trial function $\psi_t = e^{-ks+ct}$ with k and c variational parameters. The general remarks made previously (for the case $\alpha = 0$) also apply here. The optimum value of α depends on Z. In Table I may be found the optimum values of α together with the lowest eigenvalues for all two electron atoms up to $Z = 9$. As for the previous case, the error is more or less independent of Z. The least error is made for $Z = 9$: less then 1/10 of 1% percentage error is made for $Z = 1$, for which we see that the H^- atom is barely bound. However the corresponding eigenfunction ϕ_o as given by (20) is by no means the best simple trial function for H^-. Chandrasekhar[8] obtained $E_o = 0.5133$ with a trial function of the form $\psi_t = e^{-ks} \cosh ct$. Such a function is not readily generalized in a simple way. The difficulty really stems from the Pauli principle: ψ must be even (for the $'S$ states) or odd (for the ^3S states) in the variable t. To generalize this in a simple manner requires the assumption

$$(21) \qquad \psi_t = \phi(s + \beta t) \pm \phi(s - \beta t) \, .$$

Assumption (21) is really an example of Fock's method[9] in a slightly different guise and experience shows that it leads to an integro-differential equation for ϕ. It may be that the two-body assumption made here is sufficiently good to make it worth-while to solve this equation numerically. A more important reason for considering this equation is that a similar assumption is necessary to obtain a good representation of the excited states[6].

4. Suggestions for improvement

Can we generalize the effective two-body method here introduced and still retain the simplicity of solution of the final equation? It appears that the assumption $\psi_t = \phi(s)\, G(\frac{u}{s}, \frac{t}{u})$ where G is any prescribed (square integrable) function of the variables indicated, leads to essentially the variational principle (11), with different values of the numerical coefficients for different choices of G. This is easy to see because $\int_o^s du \int_u^u dt$ takes on constant limits in terms of the new variables. However, Kinoshita[5] has shown that an exact power series solution of the ground state wave function of the helium atom would not contain terms of the form $(\frac{u}{s})^n (\frac{t}{u})^m$ where n, m are positive integers. Therefore, the additional freedom of choosing the function G would not appear to be useful, even in the variational principle. An improvement in accuracy naturally requires the introduction into the wave function of the dependence on the variables u and t. A natural attempt to improve the results of the two-body method is to let

$$\psi_t = \phi(s)\,\chi(u,t) \tag{22}$$

with $\phi(s)$ prescribed, and to solve the resulting Euler equation for χ. Such an assumption may be viewed as an 'enforced' separation of variables. There would result a Schrödinger equation in only the two independent variables u and t. One might hope to get some insight in this manner into the dependence of the time wave function on these variables. It is simpler to restrict χ to be a function of u or t above, in which case it too becomes an effective two-body wave function. For example, to improve the ground state wave function $\phi_o(s)$, let

$$\psi_t = e^{-k\,s/2}\,\chi\,(u)\,. \tag{23}$$

With distances normalized by k, there results, after integration over t and s

$$\delta\int_o^\infty du\cdot u^2\left\{a(u)\left(\frac{d\chi}{du}\right)^2 - b(u)\,\chi\,\frac{d\chi}{du} + \frac{a(u)}{4}\,\chi^2 - \frac{1}{k}\left[Zv(u) - \frac{a(u)}{4u}\right]\chi^2 - \frac{E}{k^2}\,a(u)\,\chi^2\right\} = 0 \tag{24}$$

where
$$a(u) = e^{-u}(1+u+u^2/3)\;,$$
$$b(u) = e^{-u}(u+u^2)/3\;,$$
$$v(u) = e^{-u}(1+u)\;.$$

Setting $\chi(u) = a^{-1/2}F(u)$, the Schrödinger equation for F is

$$\frac{d^2F}{du^2} + \frac{2}{u}\frac{dF}{du} + \left[\frac{E}{k^2} - \frac{1}{4} + c(u) + \frac{1}{k}\left(Z\,\frac{v(u)}{a(u)} - \frac{1}{4u}\right)\right]F = 0 \tag{25}$$

subject to the normalization condition $\int_0^\infty du\, F^2 \cdot u^2 = 1$. The function

$$c(u) = \frac{1}{36}\,\frac{12+u^2(1+u)^2}{(1+u+u^2/3)^2}$$

is fairly constant over the entire range of u. This equation is reminiscent of the sort of inter-atomic potentials occurring in molecules, but it appears that it would have to be solved numerically. As in the Ritz method, the optimum value of k has to be determined by variation, and the value given by (14), say, is not necessarily the best one. It is perhaps worth observing that the asymptotic form of the equation for F for large values of u is again hydrogenic.

In a similar manner, the assumption

$$(26) \qquad \psi_t = e^{-\frac{k}{2}s}\chi(t)$$

results in

$$(27) \qquad \delta\int_0^\infty dt\,\left\{a(t)\left(\frac{d\chi}{dt}\right)^2 - \frac{1}{k}\,v(Z,t)\,\chi^2 - a(t)\left(\frac{E}{k^2} - \frac{1}{4}\right)\chi^2\right\} = 0$$

where $a(t) = (3 + t^2)\cosh t - 3t\sinh t$,

$v(Z,t) = (\frac{3}{2} - Z)\cosh t + (Z - 1)t\sinh t$.

In deriving this, we have made use of the fact that $\chi(t)$ must have a prescribed symmetry (even-ness for 'S states) in the variable t. Letting $\chi(t) = ta^{-1/2}F(t)$, there results

$$(28) \qquad \frac{d^2F}{dt^2} + \frac{2}{t}\frac{dF}{dt} + \left[\frac{E}{k^2} - \frac{1}{4} + c(t) - \frac{1}{k}\frac{v(Z,t)}{a(t)}\right]F = 0$$

with $c(t) = \frac{1}{4}(\frac{a'}{a})^2 - \frac{1}{2}\frac{a''}{a}$, and subject to the boundedness of $\int_0^\infty dt\cdot t^2F^2$.

It would be interesting to solve numerically either (25) or (28) in order to compare with some of the known variational calculations. No doubt, it is too much to expect to improve upon Kinoshita's work in this manner because even though we have (in comparison with assumption (9)) retained all powers of u and t (or both, if assumption (22) is used), we have neglected additional powers of s. However, compared with two-electron calculations which have not been so extensive, it is quite possible that this procedure may be the simplest way to get very good approximate results. If the n^{th} eigenstate is desired, than of course $\phi_n(s)$ in (22) should be specified, and the resulting equation for χ should be solved for its nth eigenstate. Finally, we mention that we may combine the method of Section 2 with the method above (restricting χ to be a function of t above) to obtain dependence of the trial wave function on all three variables.

Appendix

The radial equation for a hydrogenic atom with charge number Z and orbital quantum number λ is

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \left[2E + \frac{2Z}{r} - \frac{\lambda(\lambda+1)}{r^2}\right]R = 0 \text{ .}$$

The eigenfunctions for the bound states are

$$R_u = \rho^{\lambda} e^{-\frac{\rho}{2}} L_n^{\lambda}(\rho)$$

where

$$\rho = 2kr$$

$$2E = - k^2$$

and L_n^{λ} is the generalized Laguerre function[10]

$$L_n^{\lambda}(\rho) = \sum_{j=o}^{n} \binom{n+\lambda}{n-j} \frac{(-\rho)^j}{j!} \text{ .}$$

They satisfy the relationship

$$n!\, L_n^{\lambda}(\rho) = e^{\rho}\rho^{-\lambda} \frac{d^n}{d\rho^n} (e^{-\rho}\rho^{n+\lambda}).$$

The first few generalized Laguerre functions for fixed λ are

$$L_o^{\lambda}(\rho) = 1$$

$$L_1^{\lambda}(\rho) = \lambda + 1 - \rho$$

$$L_2^{\lambda}(\rho) = \frac{1}{2}\left[(\lambda+1)(\lambda+2) - 2(\lambda+2)\rho + \rho^2\right] \text{ .}$$

The associated eigenvalues are $E_n = - \frac{1}{2} \frac{Z^2}{(n+\lambda+1)^2}$.

In the notation used here, n is the radial quantum number and not, as is frequent usage, the total quantum number $(n+\lambda+1)$.

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